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Renormalization of Coulomb interactions in s-wave superconductor Na_xCoO_2

Keiji Yada [a], Hiroshi Kontani [a]

[a] *Department of Physics, Nagoya University, Furo-cho, Chikusa-ku, Nagoya, 464-8602, Japan*

Abstract

We study the renormalized Coulomb interactions due to retardation effect in Na_xCoO_2. Although the Morel-Anderson's pseudo potential for a_{1g} orbital μ^*_{a1g} is relatively large because the direct Coulomb repulsion U is large, that for interband transition between a_{1g} and e'_g orbitals $\mu^*_{a1g,eg'}$ is very small since the renormalization factor for pair hopping J is square of that for U. Therefore, the s-wave superconductivity due to valence-band Suhl-Kondo mechanism will survive against strong Coulomb interactions. The interband hopping of Cooper pairs due to shear phonons is essential to understand the superconductivity in Na_xCoO_2.

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Since the discovery of superconductivity in Na_xCoO_2, both theoretical and experimental studies have been actively performed to elucidate the mechanism of superconductivity and the pairing symmetry. Various theoretical studies have suggested that the development of magnetic fluctuation due to the existence of hole pockets composed of e'_g orbitals gives rise to an anisotropic superconductivity. However, such hole pockets are not observed in ARPES measurements. On the other hand, smallness of the impurity effect on T_c suggests that this system is s-wave superconductivity due to electron-phonon interaction. However, since a large repulsive force due to Coulomb interaction breaks s-wave Cooper pairs in transition-metal materials, simple s-wave superconductivity may not be favored.

In our previous paper, we studied the multi-orbital d-p model with electron-phonon interactions and found that A_{1g} mode phonons and E_g mode phonons (we call breathing and shear phonons, respectively) are strongly coupled with t_{2g} electrons[1]. Breathing phonons and shear phonons induce the intraband and the interband transition, respectively. The interband transition of Cooper pairs due to shear phonons enhances the effective attractive force as well as the transition temperature even if e'_g-like bands are valence-band. We call this mechanism the valence-band Suhl-Kondo (SK) mechanism. It is highly possible that s-wave superconductivity is realized because of the large attractive force against the Coulomb repulsion. Shear phonons as well as breathing phonons are important to understand the electron-phonon mechanism superconductivity in Na_xCoO_2.

In the present paper, we study the depairing effect due to Coulomb interactions to confirm the reality of s-wave superconductivity in Na_xCoO_2. We consider the pair hopping J and the direct Coulomb repulsion U because Na_xCoO_2 is a multi-orbital system. The effective attractive force due to breathing phonons are reduced by U and interband transition of Cooper pairs due to shear phonons are prevented by J. In this paper, we calculate the renormalized Coulomb interactions due to retardation in Na_xCoO_2, and we find out that the pair hopping J is significantly reduced.

The energy scales of electron-phonon interactions and Coulomb interactions are of the order of ω_D and W, respectively, where ω_D is the Debye frequency for phonons and W is the band width. In Na_xCoO_2, ω_D for shear phonon and breathing phonon are approximately 500 and 600 cm^{-1} ($\sim$0.06 and 0.07 eV), respectively, and the t_{2g} band width is $\sim$ 1.5 eV. Coulomb interactions have larger energy scale, so they are reduced by retardation effect. The renormalized Coulomb interactions are obtained by integrating high energy region.

$$U^*_{a1g} = U - UAU^*_{a1g} - 2JBJ^*_{a1g,eg'}, \quad (1)$$

$$U^*_{eg'} = U - UBU^*_{eg'} - JAJ^*_{a1g,eg'} - JBJ^*_{eg',eg'}, \quad (2)$$

$$J^*_{a1g,eg'} = J - JBU^*_{eg'} - UAJ^*_{a1g,eg'} - JBJ^*_{eg',eg'}, \quad (3)$$

$$J^*_{eg',eg'} = J - JBU^*_{eg'} - JAJ^*_{a1g,eg'} - UBJ^*_{eg',eg'}, \quad (4)$$

where U^*_{a1g} ($U^*_{eg'}$) is the renormalized Coulomb repulsion for a_{1g} (e'_g) orbital, and $J^*_{a1g,eg'}$ ($J^*_{eg',eg'}$) is the renormalized pair hopping between a_{1g} orbital and e'_g orbital (e'_g orbitals). A and B are the renormalization factors for a_{1g}

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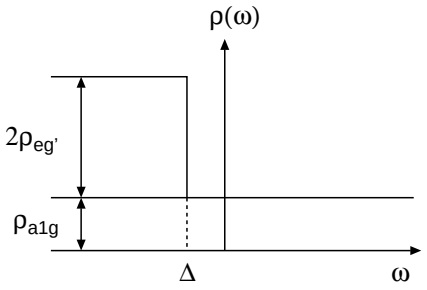

Fig. 1. DOS of Na_xCoO_2.

and e'_g orbitals, respectively.

$$A = \frac{T}{N}\sum_{\mathbf{k}}\sum_{\omega_D<|\varepsilon_\ell|<W}|G_{a1g}(\mathbf{k},i\varepsilon_\ell)|^2, \quad (5)$$

$$B = \frac{T}{N}\sum_{\mathbf{k}}\sum_{\omega_D<|\varepsilon_\ell|<W}|G_{eg'}(\mathbf{k},i\varepsilon_\ell)|^2. \quad (6)$$

We put $\omega_D = 550$ (cm^{-1}) for breathing and shear phonons, and $W = 1.5$ (eV). Na_xCoO_2 has a_{1g}-like band and two e'_g-like bands near Fermi level and the tops of e'_g-like bands Δ are located below Fermi level. So we assume that the density of states (DOS) in Na_xCoO_2 has step as shown in Fig. 1. We put $\rho_{a1g} = 0.38$, $\rho_{eg'} = 0.65$, which is derived from the value of DOS near Fermi level in the lattice model[2]. Then, A and B are calculated from Eq. 5 and Eq. 6, respectively, $A = \rho_{a1g}\log(W/\omega_D) \approx 1.2, B = \rho_{eg'}\int_{\omega_D}^{W}\frac{1}{\varepsilon}(\frac{1}{2}+\frac{1}{\pi}\mathrm{Arctan}(\frac{\Delta}{\varepsilon}))d\varepsilon$. In the case of $\omega_D \gg |\Delta|$, $B \approx \frac{1}{2}\rho_{eg'}\log(W/\omega_D) \approx 1.0$. In a realistic parameter regime $U \gg J$, we can easily solve Eq. 1∼4.

$$U^*_{a1g} \approx U/(1+AU), \quad (7)$$

$$U^*_{eg'} \approx U/(1+BU), \quad (8)$$

$$J^*_{a1g,eg'} \approx J/(1+AU)(1+BU), \quad (9)$$

$$J^*_{eg',eg'} \approx J/(1+BU)^2. \quad (10)$$

Since the renormalization factor for J is square of that for U, J is significantly renormalized. When we put $U \approx W = 1.5$ (eV), $U^*_{a1g}/U \approx 1/2.8$ and $J^*_{a1g,eg'}/J \approx 1/7$. Fig. 2 shows the renormalized Coulomb interactions which is calculated from Eq. 1∼4 for $U = 10J = 1.5$ (eV) and $U = 4.5$, $J = 0.3$ (eV). The latter value of U and J is predicted by the ab-initio calculation[3]. The Δ-dependence of U^*_{a1g} is very small because the renormalization factor A is constant. However, $U^*_{eg'}$ and J^* decrease as Δ increases. This is because the renormalization factor B increases with Δ. The Morel-Anderson's pseudo potential μ^* is obtained by multiplying U^* by DOS[4]; $\mu^* = \mu/(1+\mu\log(W/\omega_D))$, where $\mu = U\rho$. In the case of $U = 10J = 1.5$ (eV), μ^* for a_{1g} (e'_g) orbital $\mu^*_{a1g} \approx 0.2$ ($\mu^*_{eg'} \approx 0.4$). μ^* for interband transition between a_{1g} orbital and e'_g orbital (e'_g orbital) is $\mu^*_{a1g,eg'} \approx 0.01$ ($\mu^*_{eg',eg'} \approx 0.02$). $\mu^*_{a1g} \approx 0.2$ is relatively large value, because μ^* is on the order of 0.1 in normal metals. On the other hand, $\mu^*_{a1g,eg'} \approx 0.01$ is much smaller value. So the effect of Coulomb interactions on interband hopping due to shear phonon is very small.

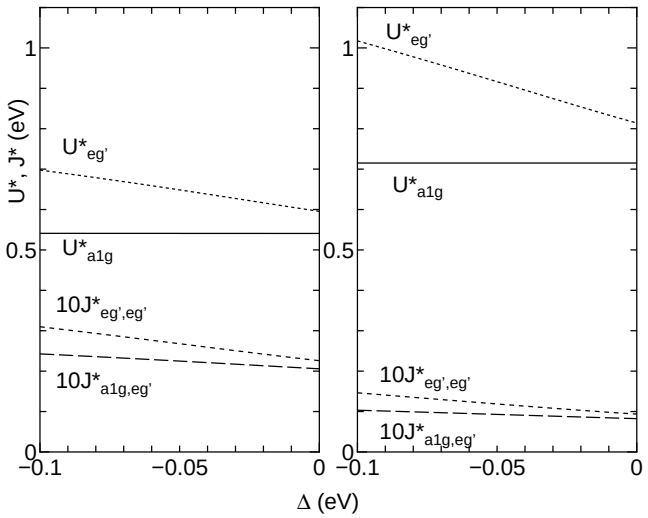

Fig. 2. Renormalized Coulomb interactions for $U = 10J = 1.5$ (eV) (left panel) and $U = 4.5$, $J = 0.3$ (eV) (right panel).

By using the same model shown in Fig. 1, we derive the transition temperature for $\omega_D \gg |\Delta| \gg T_c$ ($\Delta < 0$). $T_c \approx \omega_D \exp(-1/\lambda^*_{\mathrm{eff}})$, where λ^*_{eff} is given by

$$\lambda^*_{\mathrm{eff}} = \lambda^*_1 + \frac{2\lambda^*_2\lambda^*_3\{\frac{1}{2}\log(\frac{\omega_D}{|\Delta|})+\frac{1}{\pi}\}}{1-\lambda^*_4\{\frac{1}{2}\log(\frac{\omega_D}{|\Delta|})+\frac{1}{\pi}\}}, \quad (11)$$

where $\lambda^*_1 \sim \lambda^*_4$ are the attractive force induced by electron-phonon coupling. The expression of $\lambda^*_1 \sim \lambda^*_4$ are written in ref. [1]. The second term in the right-hand side is the SK term. Although relatively large μ^*_{a1g} and $\mu^*_{eg'}$ reduces λ^*_1 and λ^*_4, λ^*_2 and λ^*_3 hardly change because $\mu^*_{a1g,eg'}$ takes a very small value. Therefore, λ^*_{eff} can be positive value even in the case of λ^*_1 is negative value because SK term remains a relatively large positive value. This means that the superconductivity due to SK mechanism is possible even if the attractive force due to breathing phonons cancel out by a large Coulomb repulsion.

In conclusion, we study the renormalized Coulomb interactions U^* and J^* in a multi orbital system which describes the t_{2g} band of Na_xCoO_2. The pair hopping J is significantly renormalized by the retardation effect, and the effect of J^* on interband hopping due to shear phonon is very small. Therefore, valence-band SK mechanism works even if we consider the strong Coulomb interactions. The interband hopping of Cooper pairs due to shear phonons is essential in understanding the superconductivity in Na_xCoO_2.

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